Using Evolutionary Algorithms to Induce Oblique Decision Trees

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Abstract

This paper illustrates the application of evolutionary algorithms (EAs) to the problem of oblique decision tree induction. The objectives are to demonstrate that EAs can find classifiers whose accuracy is competitive with other oblique tree construction methods, and that this can be accomplished in a shorter time. Experiments were performed with a (1+1) evolutionary strategy and a simple genetic algorithm on public domain and artificial data sets. The empirical results suggest that the EAs quickly find competitive classifiers, and that EAs scale up better than traditional methods to the dimensionality of the domain and the number of training instances.

1 INTRODUCTION

Decision trees (DTs) are popular classification algorithms, and there are numerous algorithms to induce a tree classifier from a given set of data (Murthy,). Most of the tree inducing algorithms create tests at each node that involve a single attribute of the data. These tests are equivalent to hyperplanes that are parallel to one of the axis in the attribute space, and therefore

the resulting trees are called axis-parallel. These simple univariate tests are convenient because a domain expert may interpret them easily, but they may result in complicated and inaccurate trees if the data can be partitioned by hyperplanes that are not axis-parallel. Oblique decision trees use multivariate tests that are not necessarily parallel to an axis, and in some domains may result in much smaller and accurate trees. However, these trees are not as popular as the axis-parallel trees because the tests are harder to interpret, and the problem of finding oblique hyperplanes is more difficult than finding axis-parallel partitions.

The purpose of this paper is to illustrate the application of EAs to the task of oblique decision tree induction. The objectives are to show that, in some domains, evolutionary optimization may result in classifiers whose accuracy is competitive with other oblique tree construction methods, and that this can be accomplished in shorter time. The results of our experimental study suggest that the EA-augmented inducers can quickly find competitive classifiers, and that they scale up better than traditional oblique DT inducers to the size and dimensionality of the training sets.

The paper is organized as follows. The next section provides a brief background on oblique decision trees and a brief review of relevant previous work. Section 3

describes some of the advantages of using EAs to find splits in oblique DTs, and describes our approach to this problem. Section 4 has experimental results that illustrate the advantages of the evolutionary approach using public domain and artificial data sets. Finally, section 5 has a brief summary and the conclusions of the paper.

2 OBLIQUE DECISION TREES

The task of any DT inducer is to use the information contained in a training set of labeled instances to create a model that predicts the class of unseen instances. In this paper, we consider that the instances take the form $(x_1, x_2, ..., x_d, c_j)$, where the x_i are real-valued attributes, and the c_j is a discrete value that represents the class label of the instance. As was mentioned in the introduction, most tree inducers consider tests of the form $x_i > k$ that are equivalent to axis-parallel hyperplanes in the attribute space. The task of the inducer is to find appropriate values for i and k. In this paper we consider more general tests of the form

$$\sum_{i=1}^{d} a_i x_i + a_{d+1} > 0, \tag{1}$$

where the a_i are real-valued coefficients. In this case, the task of the inducer is much harder than before, because it involves searching in a d+1-dimensional space. It has been shown that finding the best oblique tree is NP-complete (Heath, Kasif, & Salzberg, 1993), and therefore existing oblique DT inducers use some sort of greedy search to find values for the coefficients. To evaluate the candidate hyperplanes, these search algorithms use a heuristic measure of the impurity of the test. Many impurity measures have been proposed (Murthy,); each has its own advantages and

disadvantages, and each defines a different optimization problem.

Breiman, Friedman, Olshen, and Stone (1984) introduced the first algorithm to induce oblique DTs: CART with linear combinations. At each node of the tree, the algorithm iteratively finds locally optimal values for each of the a_i coefficients. Hyperplanes are generated and tested until the marginal benefits become smaller than a constant.

Murthy, Kasif, and Salzberg (1994) introduced OC1, which uses an ad-hoc combination of hillclimbing and randomization. As in CART, the hillclimber finds locally optimal values for one coefficient at a time, although OC1 offers several variants to choose the order in which the coefficients are optimized. The randomization component takes two forms: OC1 uses multiple random restarts, and when hillclimbing reaches a local minimum the hyperplane is perturbed in a random direction. Murthy et al. present OC1 as an extension of CART with linear combinations that overcomes some of its limitations. In particular, they claim that CART's deterministic nature may cause it to get trapped in local minima, and that using randomization may improve the quality of the DTs. In addition, OC1 produces multiple trees using the same data, and unlike CART the time used at each node in the tree is bounded. They present experimental results that suggest that OC1 outperforms CART in several domains.

Heath, Kasif, and Salzberg (1993) used simulated annealing to perturb the hyperplane's coefficients. Simulated annealing is a more sophisticated optimizer than those used in CART and OC1, and in some domains it can produce small and highly accurate trees. However, simulated annealing converges very slowly, and the DT inducer has to examine a large number of hyperplanes,

making it inadequate for large data sets.

Other related work in this area includes the Linear Machine Decision Trees (LMDT) system (Utgoff & Brodley, 1991; Brodley & Utgoff, 1995). The LMDT algorithm is very different from the other systems. Instead of using a test similar to equation 1, at each node the LMDT has a set of R linear discriminant functions $g_i(\mathbf{X}) = \mathbf{W}_i^T \mathbf{X}$ and assigns class $i \in \{1,...,R\}$ to the instance described by $\mathbf{X}=(x_1,...,x_d)$ if $\forall i,i \neq$ $j g_i(\mathbf{X}) > g_j(\mathbf{X})$. The training algorithm changes the weight vectors \mathbf{W}_i according to a specific correction rule, and the tree is built recursively until all the instances in a node belong to the same class. There is no need to use a heuristic to measure the impurity of each split or to decide when to stop. EAs could also be used in combination with LMDT to adapt the weight vectors, but we do not address LMDT in this paper.

3 EVOLUTIONARY OBLIQUE DTs

At the heart of DT inducing algorithms there is an optimization task: to minimize the impurity of the split defined by a hyperplane. This task is performed at each node of the tree, then the data is partitioned into subsets, and the algorithm is applied recursively to each subset. Quinlan (1986) described this procedure as 'top-down' induction of decision trees. Our proposal is to use EAs as the optimization algorithm.

Evolutionary algorithms are a promising alternative to existing oblique tree algorithms for several reasons:

More sophisticated optimizers. EAs are not limited to consider one coefficient at a time (like CART and OC1), and it is likely that EAs find better splits than the simple greedy hillclimbers that are popular.

No need for optimal splits. Finding the best split at each node does not guarantee that the best tree will be found. Therefore, there is no need to run the EAs (or any other optimizer, for that matter) until they find the best solution that they can. It is well known that EAs quickly improve on the initial solutions, and so we may use the best hyperplanes found after just a few iterations.

Scalability to high dimensional spaces. The dimension of the search space is defined by the number of attributes that describe each instance. In practice this can be a large number, and the execution time of some existing DT algorithms may not scale up well. In contrast, EAs have been shown to have good scalability properties (?).

Use of domain knowledge. There are numerous opportunities to incorporate knowledge about the DT inducing problem into the EAs. For instance, real-valued encodings and operators seem natural to represent hyperplanes. The positive experiences with existing DT inducers suggest that recombination or mutation operators that create new hyperplanes that are only slight variations of the originals may work well. This can be accomplished by restricting mating between similar hyperplanes or by using small mutation steps, for example. In addition, the execution time may be reduced using known 'good' solutions to seed the initial population. In particular, we seed the populations with hyperplanes obtained by an axisparallel algorithm.

Hybridization. Most DT algorithms use a local optimizer that is well tuned to the tree induction task, and interfacing it to the EA could boost performance significantly.

Tolerance to noise. More efficient EA-based DT inducers may be obtained by approximating the fitness of a hyperplane by using a small random sample of instances to evaluate the split. This approximation would assign different fitness values to the same hyperplane every time that it is evaluated, but EAs are tolerant such noisy fitness evaluations (Grefenstette & Fitzpatrick, 1985; Miller & Goldberg, 1996a).

Parallel implementations. It is straightforward to implement EAs on parallel computers (see e.g., (Cantú-Paz, 1998)), and the expected performance improvements are very promising.

This paper does not consider hybrids or parallel implementations, but we use knowledge about the problem in our choice of encoding and operators and to seed the initial population. The EAs were run for a fixed number of iterations that, in many cases, were not enough for the EA to converge to a unique solution or to find the best hyperplane that it could, but that were sufficient to reach acceptable solutions. In addition, we performed experiments to explore the scalability of EAs and their sensitivity to sampling.

4 EXPERIMENTS

To demonstrate the feasibility of using EAs to search for oblique partitions, we conducted three sets of experiments. In the first set, we used the same four public-domain data sets used by Murthy et al. (1994) to evaluate OC1. Next, we used artificial data with known properties, and we perform experiments to study the scalability of the different algorithms to the dimensionality of the domain. Finally, we present experiments with a larger database to illustrate how sampling may help to scale up the evolutionary approach

to more realistic situations.

The experiments compare the performance of two baseline DT inducers against two inducers that use EAs. The first baseline DT system is OC1 with its default parameters, and the second is OC1 limited to axis-parallel partitions, which we call OC1-AP.

The first DT system with an EA is an extension of OC1 that uses a (1+1) evolutionary strategy with self-adaptive mutations. We call this OC1-ES. The candidate hyperplane is represented as a vector of real-valued coefficients, $a_1, ..., a_{d+1}$, and for each coefficient there is a corresponding mutation step $\sigma_1, ..., \sigma_{d+1}$, which are initially set to 1. At each iteration, the mutation steps are updated and a new hyperplane is obtained according to the following rule:

$$\nu = N(0, 1)$$

$$\tilde{\sigma}_i = \sigma_i \exp(\tau' \nu + \tau N(0, 1))$$

$$\tilde{a}_i = a_i + \tilde{\sigma}_i N(0, 1),$$
(2)

where N(0,1) indicates a realization of a unit normal variate, $\tau = (\sqrt{2\sqrt{d}})^{-1}$, and $\tau' = (\sqrt{2d})^{-1}$. The first hyperplane is the best axis-parallel split found by OC1.

The second extension of OC1 with an EA uses a simple generational GA with real-valued genes, and is called OC1-GA. The GA used pairwise tournament selection, uniform crossover with probability 1.0, and no mutation. The population size was set to $20\sqrt{d}$, along the lines of a population-sizing theory that proposes that the population size required to reach a solution of a particular quality is $O(\sqrt{d})$ (Harik & Lobo, 1999). The best axis-parallel hyperplane was copied to 10% of the initial population, and the remainder of the population was initialized randomly.

The execution times were measured on a 500 MHz Pen-

Name	Task Description	Attributes	No. of Instances
Cancer	Diagnose a tumor as benign or malignant	9	683
Diabetes	Detect presence of diabetes	8	768
Housing	Predict housing values in suburbs of Boston	12	506
Iris	Classify type of iris	4	150

Table 1: Descriptions of the small public domain data sets used in the experiments.

Algorithm	Parameter	Cancer	Diabetes	Housing	Iris
-	Accuracy	96.2(1.0)	74.1(2.0)	82.8 (2.0)	95.5(1.8)
OC1	Leaves	3.3(1.1)	5.7(2.1)	7.3(2.6)	3.5(0.2)
	Time	28.4 (8.7)	33.0 (1.4)	19.8(1.3)	1.2(0.1)
	Accuracy	94.7(0.7)	74.0(1.0)	82.2(1.0)	92.8(2.6)
OC1-AP	Leaves	9.4(2.6)	18.9 (8.7)	10.0~(6.6)	5.2(1.4)
	Time	0.2(0.0)	0.4(0.0)	0.3(0.0)	$0.1\ (0.0)$
	Accuracy	95.2(0.9)	$73.7\ (1.4)$	82.8 (1.2)	96.3(1.5)
OC1-ES	Leaves	5.2(2.2)	17.1(5.0)	11.5 (5.7)	3.5 (0.4)
	Time	5.1(0.4)	14.0 (0.3)	8.6(0.3)	0.9(.1)
	Accuracy	94.3(0.5)	73.9(1.3)	82.4(1.1)	93.6(1.3)
OC1-GA	Leaves	9.6(2.1)	19.0 (11.6)	12.5 (5.2)	4.3(1.4)
	Time	7.7(0.4)	13.0(0.3)	8.5(0.4)	0.37(0.04)

Table 2: Comparison of different algorithms on the small public domain data sets.

tium III PC with 128 Mb of RAM running NT 4.0. The programs were compiled with the ecgs compiler version 2.91 using -O optimizations.

All experiments measure the impurity of a split using the twoing rule (Breiman et al., 1984) that is the default in OC1. The impurity was used without modifications as the fitness of the hyperplanes.

4.1 SMALL DATA SETS

The first round of experiments use small public domain data sets, which are available at UCI's machine learning repository (Blake & Merz, 1998). These are briefly described in table 1, and have been used in numerous studies of machine learning and data mining algorithms. For our comparison we follow the experimental procedure that Murthy et al. (1994) used to compare OC1 to other DT inducers: we use the stan-

dard parameters of OC1, and the results presented (in table 2) are the average of ten five-fold cross-validation experiments (50 trees total). We report the percentage of instances classified correctly, the size of the tree measured by the number of leaves, and the execution time of the program measured in seconds, along with their standard deviations (in parenthesis).

From the table it is clear that the differences in the accuracy of the different algorithms is very small. There are significant differences (at least at the 0.05 confidence level) on the cancer and iris data, but the magnitude of the differences is still small. For the four data sets, the average size of the trees found by the GA-augmented inducer was close to the axis-parallel algorithm, but in three cases (cancer, housing, and iris) OC1-ES found trees comparable to OC1. The largest differences are in execution times; the EAs be-

ing on average approximately 3 times faster than OC1, but much slower than OC1-AP.

4.2 ARTIFICIAL DATA

The next set of experiments used three artificial data sets. The purpose of these experiments is to ensure that the concept to be learned matches the bias of the algorithms (the classes are separable by oblique hyperplanes). In addition, we performed experiments to explore the scalability of the algorithms as the number of attributes varies. The three data sets were also used by Murthy et al. (1994) in their evaluation of OC1, but we used them to study different properties of the algorithms.

The first artificial data set has 2000 instances divided into two classes. Each instance has d attributes whose values are uniformly distributed in [0,1]. The data is separable by the hyperplane $x_1 + ... + x_{d/2} < x_{d/2+1} + ... + x_d$, where $d \in \{10, 20, 50\}$. These data sets are labeled LS10, LS20, and LS50 according to their dimensionality.

We followed the same experimental procedure as in the previous experiments, and the results are summarized in table 3¹. In this case, OC1-AP consistently found the least accurate and largest trees. Of course, it was the fastest algorithm, but its accuracy is too low to consider AP trees competitive (consider that random guessing would result in a 50% accuracy and the accuracy of OC1-AP on LS50 is 58%). OC1 produces the most accurate trees for LS10, but as the number of dimensions increases its performance seems to drop below the EA-augmented inducers. OC1-GA maintains the highest accuracy, but its time seems to increase

faster than OC1-ES. In any case, the EA inducers are faster than OC1 (approximately between 2x and 6x). The size of the trees found by OC1 and OC1-ES increases with the number of dimensions, but those of OC1-GA seem to remain of a constant size. However, consider that the ideal tree for this domain has two leaves, and all the algorithms find much larger trees.

The second and third artificial data sets, POL2 and RCB2, represent concepts that are supposed to be more difficult to learn. They are defined in 2-D $(x_1, x_2 \in [0, 1])$, and depicted in figure 1. The concept represented by the POL2 data is a set of four parallel oblique lines (hence its name), it contains 2000 instances divided into two classes. The "rotated checker board" (RCB2) data also has 2000 instances, but in this case they are divided into eight classes. We used the same experimental setup as before, and the results are in table 3.

In these two domains, OC1 and OC1-ES produced the most accurate and smallest trees. The smallest trees for POL2 and RCB2 have five and eight leaves, respectively, and OC1 consistently found trees of those sizes. As expected, the AP trees are the largest and least accurate, but OC1-GA found only slightly more accurate and smaller trees. Both of the EA inducers were approximately eight times faster than OC1, but in these two problems the overall performance of the ES was much better than the GA.

4.3 OPTICAL DIGIT RECOGNITION DATA

To study the problem of scalability to larger data sets, we experimented with a the optical digit recognition data set, which is also available at UCI's ML repository. This data set has 3823 instances in a training set and 1797 in a testing set; each instance is described by

¹Our results with the LS10 data are different from Murthy et al.'s because we used OC1's default pruning option (using 10% of the data), but they did not prune the resulting trees.

Algorithm	Parameter	LS10	LS20	LS50	POL2	RCB2
_	Accuracy	97.1(0.4)	88.5(1.1)	72.5(1.3)	99.6(0.1)	99.0 (0.1)
OC1	Leaves	5.3(2.2)	5.9(2.7)	10.0(3.6)	5.0(0.0)	8.4 (0.3)
	Time	170.9(12)	391.5(16.6)	608.7(32.8)	36.0(2.3)	44.8 (1.5)
	Accuracy	73.0(1.5)	64.6 (0.8)	58.6 (1.0)	94.2(0.6)	92.8(0.4)
OC1-AP	Leaves	86.7 (16.5)	71.5(29.0)	58.0 (20.8)	$77.7\ (10.4)$	85.9 (6.8)
	Time	1.6(0.0)	3.5 (0.1)	11.7(0.6)	0.3(0.0)	0.4(0.0)
	Accuracy	93.7(0.8)	87.0 (1.0)	78.5(1.6)	99.4(0.3)	98.1(0.3)
OC1-ES	Leaves	9.9(2.8)	14.4 (5.6)	16.3 (9.4)	6.3(1.2)	10.9(1.9)
	Time	29.8(2.4)	65.1(3.3)	163.9 (14.9)	4.5(0.4)	6.0(0.4)
OC1-GA	Accuracy	95.4(0.6)	$92.0\ (0.7)$	85.2(1.0)	95.3(0.4)	93.8 (0.7)
	Leaves	8.8 (3.8)	9.8 (5.9)	9.5(5.6)	57.5 (10.5)	64.6 (9.7)
	Time	36.3(3.8)	101.5(4.8)	333.3 (22.2)	4.7(0.3)	$5.0\ (0.2)$

Table 3: Comparison of different algorithms on the artificial data sets.

64 numeric attributes. The objective is to identify the instances as one of 10 digits.

With this domain, we illustrate a more realistic application of EAs to the problem of oblique DT induction. The larger size of the training set could cause fitness evaluations to be prohibitively expensive, and therefore we seek to obtain faster approximate evaluations by sampling the training set. We consider two ways of sampling. The first is a preprocessing step in which the training set is sampled once at the beginning of an experiment. This static sampling ignores all the instances that were not selected originally, possibly wasting valuable information. However, static sampling is valuable because it simulates a situation when not much data is available for training (which is usually the case in the domains that interest us). The second way of sampling is to choose a fraction of the instances available at each tree node every time a hyperplane is evaluated. This method is slightly more expensive, but it is advantageous especially when samples are small, because repetitive sampling eventually considers all the available labeled instances. Evaluating the hyperplanes with dynamic samples also means that every time that a hyperplane is evaluated its fitness is different. Repeated evaluations of the same hyperplane would enable us to better estimate its fitness (e.g., by taking the average of multiple evaluations), and some recent theory could be used to determine the optimal number of repetitive evaluations that would minimize the execution time of the GA (Miller & Goldberg, 1996b). As a first cut, however, we decided to use a single evaluation as a crude (but fast) estimate of fitness.

The results with repetitive sampling are reported in table 4. In this case, we report the average of 10 experiments, and training and testing used the partition of the instances as in the UCI repository. The algorithms use the same parameters as before. Sampling decreases the execution time as desired, but it also affects the accuracy. For each sample size, the GA finds the smallest and most accurate classifiers, and in most cases it is faster than the original oblique OC1. The ES is the fastest of the oblique classifiers, and its accuracy is better than OC1, but not as good as the GA. Note, however, that the axes-parallel OC1 is the fastest algorithm, and that its accuracy is similar to OC1-ES. In fact, using OC1-AP with the entire data set is faster and more accurate than the GA on 5%

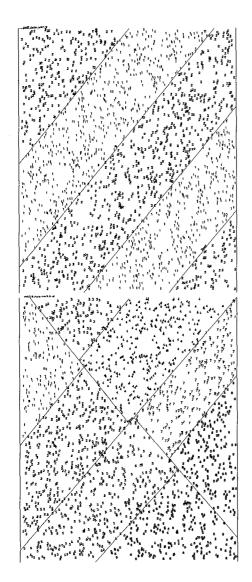


Figure 1: The POL2 and RCB2 data sets.

samples, so if the end user does not care about the relatively small differences in accuracy, in this domain axes-parallel DTs would be a good choice. If accuracy or tree size is a premium, then OC1-GA would be the best option.

In separate experiments we encountered that repetitive sampling gives more accurate results than static sampling at the beginning of the experiments. For samples of 25% or more of the training set, the accuracy was only slightly lower than with repetitive sampling ($\approx 4-5\%$), but for smaller samples, the accuracy was between 6 to 22% lower. The general trends were the same as with repetitive sampling, so we omit those results.

5 SUMMARY AND CONCLUSIONS

Traditional DT inducers use some form of heuristic greedy search to find appropriate splits. In this paper, we substitute that greedy search with two evolutionary algorithms: a (1+1) evolutionary strategy and a simple GA. We performed experiments on public domain and artificial data sets with different characteristics to evaluate the performance of the EA-based tree inducers. The results suggest that EAs are capable of finding oblique trees with similar accuracy to OC1, and that this can be done at a fraction of the cost. The experiments also suggest that the EAs scale up better than traditional methods to the dimensionality of the data.

We evaluated the use of sampling to further reduce the execution time of the inducers. Sampling resulted in faster training times, but also in a loss of accuracy, which was more pronounced when the training set was sampled statically.

This paper is only a first step in the application of

Algorithm	Parameter	5%	10%	25%	50%	100%
OC1	Accuracy	$42.1\ (7.9)$	53.7 (8.1)	74.3(2.2)	82.3(1.1)	86.4(0.9)
	Leaves	56.7(11.4)	88.5(26.0)	138.7 (69.2)	147.6 (47.1)	53.7 (30.6)
	Time	7.8(0.3)	16.6(0.7)	49.4(2.6)	$117.1\ (7.0)$	298.6 (11.1)
OC1-AP	Accuracy	68.3(2.4)	76.0(2.3)	79.4(1.3)	82.2(2.2)	84.5 (1.9)
	Leaves	22.8(4.3)	44.7(16.0)	$68.6\ (27.6)$	107.6 (20.3)	125.8 (48.2)
	Time	0.6 (0.0)	0.8(0.0)	1.4(0.0)	2.5(0.0)	5.5(0.2)
OC1-ES	Accuracy	69.8(2.0)	76.6(2.4)	82.8(1.3)	84.6 (1.4)	87.9 (1.0)
	Leaves	$17.9\ (2.9)$	28.5 (6.8)	$48.4\ (16.7)$	$68.6\ (25.9)$	84.0 (37.6)
	Time	5.5 (0.5)	9.2(0.5)	17.5(0.8)	33.0 (1.0)	63.0(3.2)
OC1-GA	Accuracy	79.5(2.6)	83.7(2.1)	87.4(1.1)	88.9(0.7)	90.2(1.1)
	Leaves	12.7(1.6)	16.8 (4.0)	24.1(8.0)	45.3(27.2)	52.3 (34.6)
	Time	8.3(0.4)	15.2 (0.6)	$36.1\ (1.4)$	75.6(2.9)	144.2 (4.5)

Table 4: Comparison of different algorithms on the digit recognition data using sampling (5%-100% of the training set) every time a hyperplane was evaluated.

EAs to oblique DT induction, and there are multiple opportunities to expand our work. In particular, we should continue the study of scalability using larger data sets (both artificial and 'real-world'), and incorporate other algorithms such as (μ, λ) ES. Also, the domain knowledge should be exploited by designing specialized operators and by combining EAs with local hillclimbers.

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